



Quantum Computing

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Topics

- Introduction
- Quantum Information and Quantum Computers
- State Description
- Quantum Mechanics: Mathematical Model of the Physical World
- Qubits and Their Physical Realization
- Quantum Gates and Quantum Circuits
- Quantum Cellular Automata
- Conclusions



Introduction

- As solid-state technology continues to improve at a very fast pace physical limitations of current computational models are becoming more of a concern.
- If there is a minimum amount of power dissipated for the execution of a logical step, then the faster computers become, more power is needed for operation.
- In recent times, alternatives to traditional computing are being studied.

Introduction

- At present there are two basic directions on the intersection of modern physics, computer science, and material science:
 1. The traditional approach - squeezing more devices on a computer chip (VLSI) while fighting the increasing undesirable quantum mechanical effects (leakage currents, etc.)
 2. Designing new devices to take advantage of quantum mechanical effects, and also considering the implementation of quantum computing systems
- Richard Feynmann of MIT has speculated that computation can be done more efficiently by using quantum effects.
- He has suggested that problems for which polynomial time algorithms do not exist could be solved.
- Further, these algorithms could possibly be made reversible.

Quantum Information and Quantum Computing

- Concerned with the transmission and processing of quantum states and the interactions of such quantum information with the “classical” one.
- A quantum bit, or *qubit*, is a quantum system used to store information.
- Compared to the classical bit, which takes on one of two states (0 or 1), the qubit can exist in a continuum of states.
- We can measure the value of a classical bit with certainty without affecting its state.
- However the result of measuring a qubit is non-deterministic and the measurement alters its state.



Quantum Information and Quantum Computing

- “*The path from classical information to quantum information is a process of extension, refinement, and completion of our knowledge.*”
- Follows the evolution of our thinking in other areas of science
- For example consider evolution of number theory:
 - Positive numbers
 - Additive inverse of positive numbers – negative integers
 - Multiplicative inverse of integers – rational numbers
 - Irrational numbers
 - Real number system



Quantum Information and Quantum Computing

- Quantum computers are stochastic engines since the state of the quantum system is uncertain.
- A certain probability is associated with any possible state the system can be in.
- The output states of a stochastic engine are random: the label of the output cannot be discovered.
- All that can be done is label a set of pairs consisting of an output state of an observable and a measured value of that observable.
- Mathematically, in quantum mechanics, each pair consists of an eigenstate of a Hermitian operator and its corresponding eigenvalue.



Quantum Information and Quantum Computing

- While a classical bit can be in one of two states, 0 or 1, a qubit can be in states $|1\rangle$ or $|0\rangle$, which are *computational basis states*, or in any state which is a linear combination of these.
- Considering a system with n qubits, whose individual states are described by vectors in a 2D space:
 - The possible states of the quantum system of n particles form a vector space of 2^n dimensions.
 - With n qubits, 2^n n -tuples can be constructed and a system with 2^n states can be described.
- Even though a qubit can be in one of infinitely many superposition states (combination of basis states) when a qubit is “measured” the measurement changes the state of the quantum system to one of the two basis states.
- From one qubit we can only extract a single classical bit of information.

Quantum Information and Quantum Computing

- In designing quantum algorithms a major problem that needs to be overcome is *decoherence* – the process of disturbing the quantum state through the interaction with the environment.
- Access to results of a quantum system must be restrictive.
- *Entangled state* – two photons or two electrons can be in a superposition state of close coupling with each other, in this intimately fused state.
- The state of an entangled system cannot be decomposed into individual contributions of each particle.
- Two quantum particles may be in an entangled state even if they are not in close proximity to each other.
- A change of state in one particle instantaneously affects the other particle and determines its state.

Quantum Information and Quantum Computing

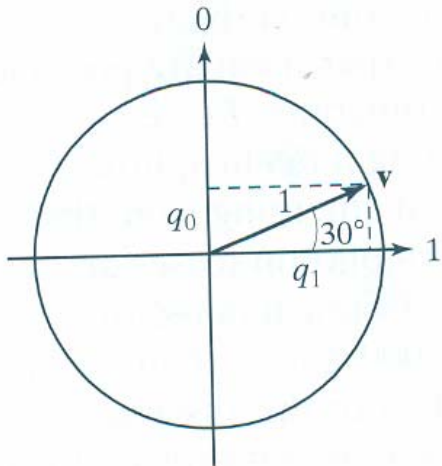
- Analogy:

“When Alice and Bob get married to each other their lives become entangled. After a few months they find out that Alice is pregnant. Shortly afterwards Bob takes off to another galaxy. The very moment Alice gives birth to their child, Bob’s state changes instantly, despite the fact that he might be light years away. Bob becomes a father. An external viewer could see the baby and decide that bob’s state has changed.”

- Electrons in the same orbital are considered entangled and follow *Pauli exclusion principle*.

State Description

- Mathematical model for the state of a two dimensional quantum system
- State can be represented by a vector connecting the origin of the coordinate system to a point on the periphery of a unit circle.



$$|v\rangle = q_0 |0\rangle + q_1 |1\rangle$$

$$|q_0|^2 + |q_1|^2 = 1$$

q_0, q_1 are called probability amplitudes

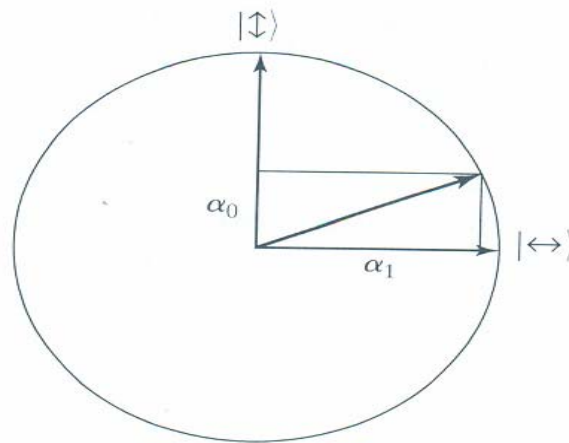
$|q_0|^2, |q_1|^2$ are probabilities of outcomes

State Description

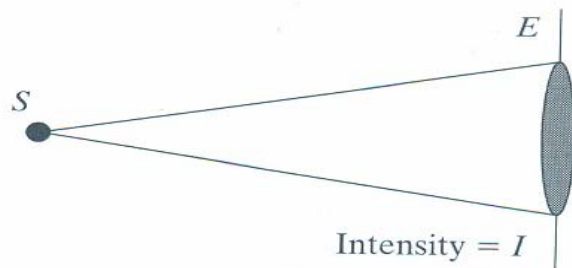
- This mathematical model can describe the photonic behaviour of light.
- Light is a form of electromagnetic radiation and can have various polarizations, for example vertical, horizontal and 45° polarizations (a superposition of vertical and horizontal states).
- Polarization of a photon can be described by the unit vector:

$$|\Psi\rangle = \alpha_0 |\updownarrow\rangle + \alpha_1 |\leftrightarrow\rangle$$

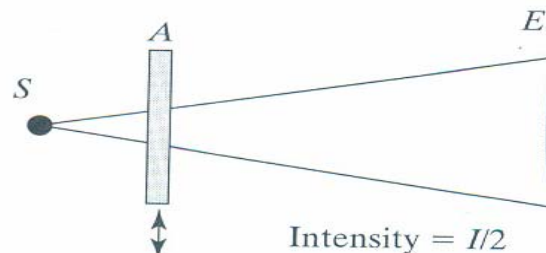
State Description



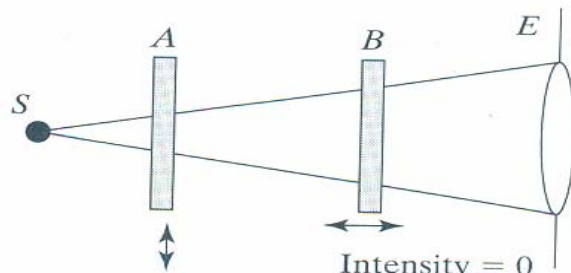
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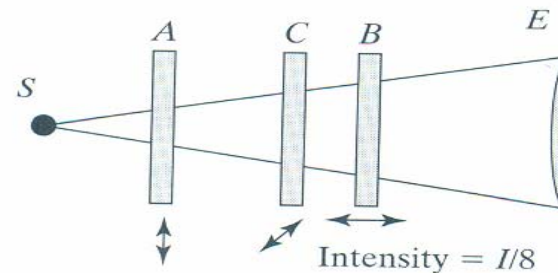
(b)



(c)



(d)



(e)



Quantum Mechanics – A Mathematical Model of the Physical World

- A good understanding of some fundamental mathematical concepts is essential in studying the new discipline of quantum computing.
- Quantum mechanics represents a mathematical model of the physical world able to explain phenomena, such as the energy spectra of atoms, which classical mechanics fails to explain.
- Important aspects:
 - Linear algebra concepts
 - Hermitian operators
 - Hilbert spaces
 - Inner products, tensor products and outer products of vectors in a Hilbert space

Quantum Mechanics – A Mathematical Model of the Physical World

- Quantum systems evolve in time.
- To capture the dynamics of a system, a mathematical model must study transformations of states represented as mathematical operators applied to vectors.
- Necessary to consider vector spaces over fields of n-dimensional complex vector space, rather than just real numbers.
- Operators, which will act as transformation matrices, must be Hermitian:

$$A^{\dagger} = (A^*)^T = A$$

Quantum Mechanics – A Mathematical Model of the Physical World

- Hilbert space is defined as an infinite-dimensional vector space with an inner (dot) product and associated norm.
- A collection of vectors $\{e_1, e_2, \dots, e_n\} \in H_n$ is called an orthonormal basis if the inner product between any two is zero, and with itself, 1.
- Using Dirac notation, vectors forming an orthonormal basis can be written as “kets”:

$$\{|0\rangle, |1\rangle, \dots, |i\rangle, \dots, |n-1\rangle\}$$

or “bras”:

$$\{\langle 0|, \langle 1|, \dots, \langle i|, \dots, \langle n-1|\}$$



Quantum Mechanics – A Mathematical Model of the Physical World

- Where:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \dots, |n-1\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

$$\langle 0| = (1 \ 0 \ \dots \ 0 \ \dots \ 0), \ \langle 1| = (0 \ 1 \ \dots \ 0 \ \dots \ 0), \dots, \langle n-1| = (0 \ 0 \ \dots \ 0 \ \dots \ 1)$$

$$|\psi\rangle = \left(\langle \psi| \right)^\dagger$$



Quantum Mechanics – A Mathematical Model of the Physical World

- An n-dimensional *ket* vector is used to describe the state of a quantum system:

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle + \dots + \alpha_{n-1}|n-1\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{n-1} \end{pmatrix}$$

- Inner product of state vector with itself is defined as:

$$\langle\psi||\psi\rangle = \begin{pmatrix} \alpha_0^* & \alpha_1^* & \dots & \alpha_{n-1}^* \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{n-1} \end{pmatrix}$$

Quantum Mechanics – A Mathematical Model of the Physical World

- A unitary operator \mathbf{U} , which is Hermitian, maps state vectors to state vectors in H_n :

$$|\Psi_b\rangle = \mathbf{U}|\Psi_a\rangle \text{ or } \langle\Psi_b| = \langle\Psi_a|\mathbf{U}$$

- Forming an operator \rightarrow e.g. construct an operator in a 2-dimensional Hilbert space H_2 whose function is to interchange the projections of a state vector

$$\alpha_0|0\rangle + \alpha_1|1\rangle \rightarrow \alpha_0|1\rangle + \alpha_1|0\rangle$$

$$\begin{aligned}\mathbf{U} &= |0\rangle\langle 1| + |1\rangle\langle 0| \\ &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} (0 \ 1) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 \ 0) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\end{aligned}$$

Qubits and their Physical Implementation

- A qubit is a mathematical model of a microscopic physical system.
- May exist in a continuum of “intermediate states” or “superpositions”
- Mathematically the physical measurement of a qubit is the projection of the state of the qubit onto its vector basis.
- Two physical systems leading to the simplest embodiments of a qubit are:
 1. The electron with two independent spin values $\pm\frac{1}{2}$
 2. The photon with two independent polarizations (e.g. vertical/horizontal)

Quantum Gates and Quantum Circuits

- Quantum gates are the building blocks of a quantum computer, just as logic gates are building blocks of a classical digital computer.
- Quantum gate transforms the state of a quantum state into a new state.
- Transformations are described by Hermitian operators, also known as a transfer matrix.
- Gates can be implemented for more than one qubit:
 - 1-qubit system = 2 possible states in H_2
 - 2-qubit system = 4 possible states in H_4
 - 3-qubit system = 8 possible states in H_8
 - n-qubit system = 2^n possible states in H_n

Quantum Gates and Quantum Circuits

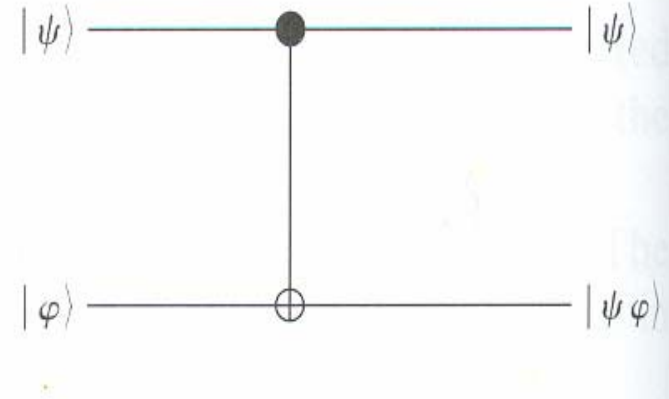
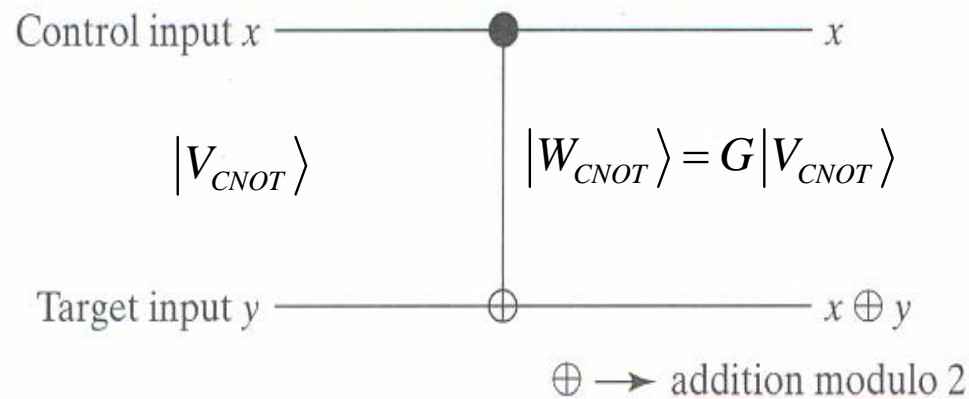
- Some important standard one-qubit transfer matrices for the system:

$$\begin{pmatrix} \alpha'_0 \\ \alpha'_1 \end{pmatrix} = (G_{2 \times 2}) \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix}$$

- The identity gate – leaves qubit unchanged $\rightarrow I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
- The X or NOT gate – transposes components of qubit $\rightarrow X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
- The Y gate – multiplies the input qubit by i and flips the two components of the qubit $\rightarrow Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
- The Z gate – changes the phase (sign flip) of a qubit $\rightarrow Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
- The Hadamard gate, H $\rightarrow H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

Quantum Gates and Quantum Circuits

- Two qubit quantum gates take in two qubits at the input and provide two outputs.
- CNOT gate (classical equivalent is an XOR gate)
- Target output is flipped if the control input is 1, otherwise target output is equal to the target input.



Quantum Gates and Quantum Circuits

- Mathematically:

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle, \quad |\varphi\rangle = \beta_0|0\rangle + \beta_1|1\rangle$$

$$|V_{CNOT}\rangle = |\psi\rangle \otimes |\varphi\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} \otimes \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} \alpha_0\beta_0 \\ \alpha_0\beta_1 \\ \alpha_1\beta_0 \\ \alpha_1\beta_1 \end{pmatrix}$$

State transformations:

$$|00\rangle \mapsto |00\rangle, \quad |01\rangle \mapsto |01\rangle, \quad |10\rangle \mapsto |11\rangle, \quad |11\rangle \mapsto |10\rangle$$

Transfer matrix G_{CNOT} is the sum of the outerproducts of the components of input and output vectors:

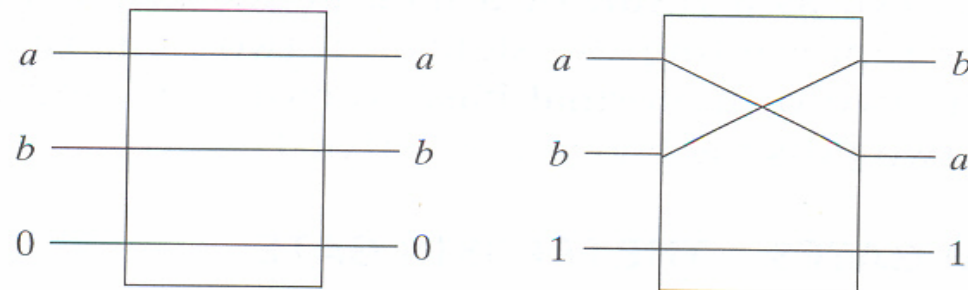
$$G_{CNOT} = |00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 11| + |11\rangle\langle 10| = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$|W_{CNOT}\rangle = G_{CNOT} |V_{CNOT}\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha_0\beta_0 \\ \alpha_0\beta_1 \\ \alpha_1\beta_0 \\ \alpha_1\beta_1 \end{pmatrix} = \begin{pmatrix} \alpha_0\beta_0 \\ \alpha_0\beta_1 \\ \alpha_1\beta_1 \\ \alpha_1\beta_0 \end{pmatrix}$$

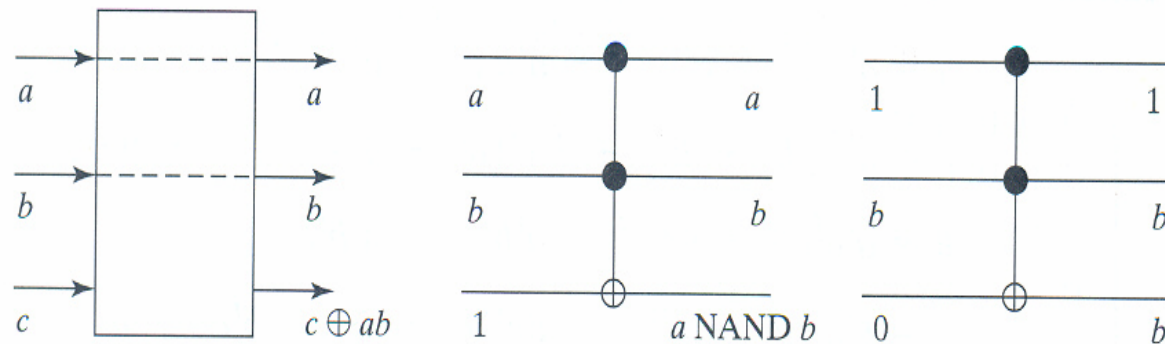
Quantum Gates and Quantum Circuits

- Some 3-qubit quantum gates:

- Fredkin Gate

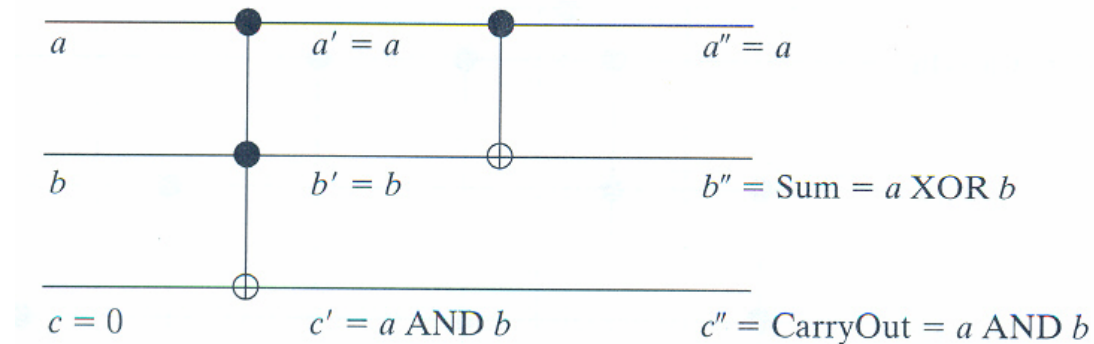


- Toffoli Gate

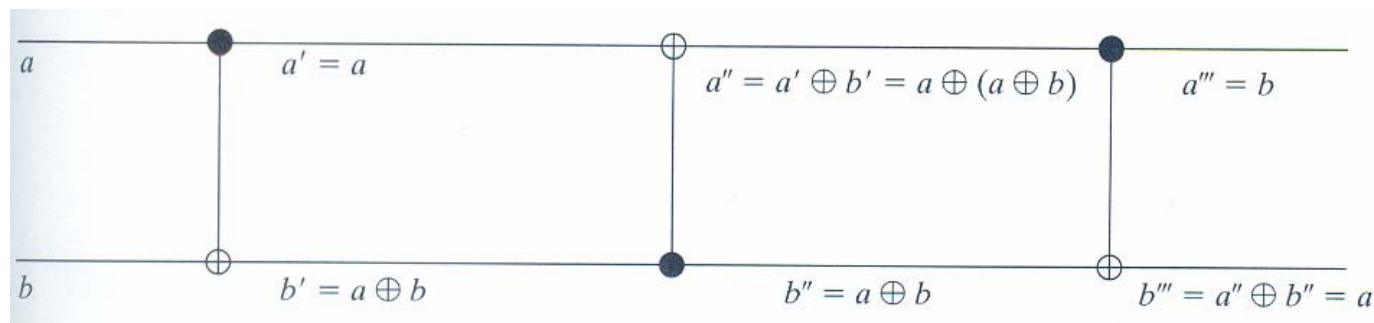


Quantum Gates and Quantum Circuits

- Some Quantum Circuits:
 - Two-bit adder made of reversible gates (Toffoli followed by a CNOT gate)



- Circuit for swapping two qubits (3 CNOT gates)





Quantum Cellular Automata

- As transistors continue to shrink, more and more quantum effects will start to overwhelm their operation.
- Presently researchers continue to try and maintain functionality of these transistors even as they get scaled down.
- Why continue the fight to maintain functionality, when it would probably be more worthwhile to find a new device that will take advantage of these quantum effects?
- A novel idea has been proposed originally by Dr. Craig Lent at University of Notre Dame – **Quantum Cellular Automata (QCA)**.



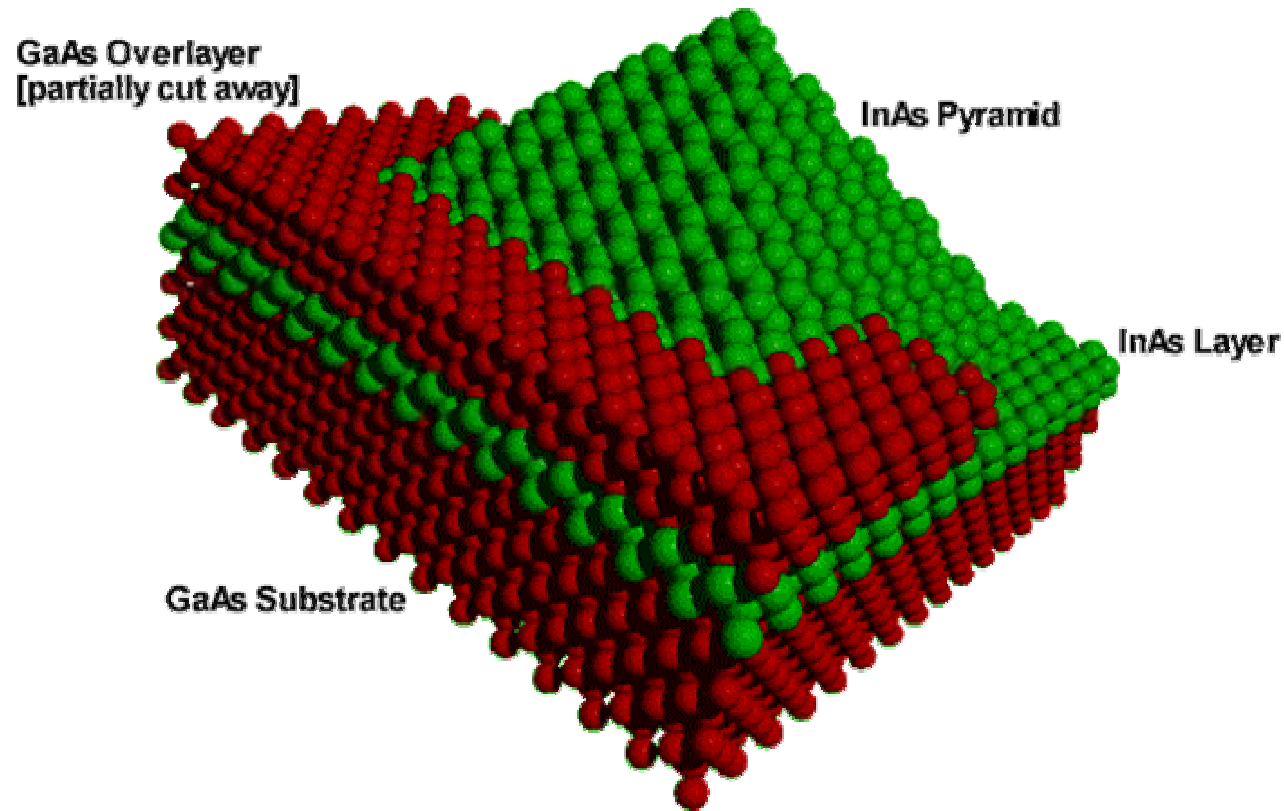
Quantum Cellular Automata

- QCA consists of planar arrays of what are called QCA cells.
- These cells have features on the very low nanometre scale.
- As features are reduced, QCA cells perform even better.
- These devices rely on quantum mechanical effects for their operation (whereas these effects hinder transistor operation).

Quantum Cellular Automata

- What is a quantum-dot?
 - Nanostructures created from standard semiconductive materials such as InAs/GaAs
 - Can be modelled and visualized as 3D quantum wells
 - Electrons once trapped inside the dot, do not alone possess the energy required to escape
 - Quantum physics is taken advantage of – the smaller a quantum dot is physically, the higher the potential energy necessary for an electron to escape

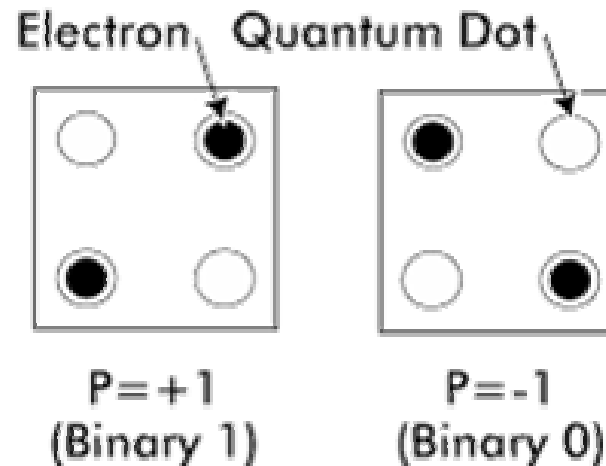
Quantum Cellular Automata



Example of a quantum dot pyramid created with InAs/GaAs
(Courtesy: University of Newcastle Condensed Matter Group)

Quantum Cellular Automata

- QCA attempts to create nanoscale computational functionality by controlling the position of single electrons.
- The fundamental QCA cell has four quantum-dots positioned at the vertices of a square.

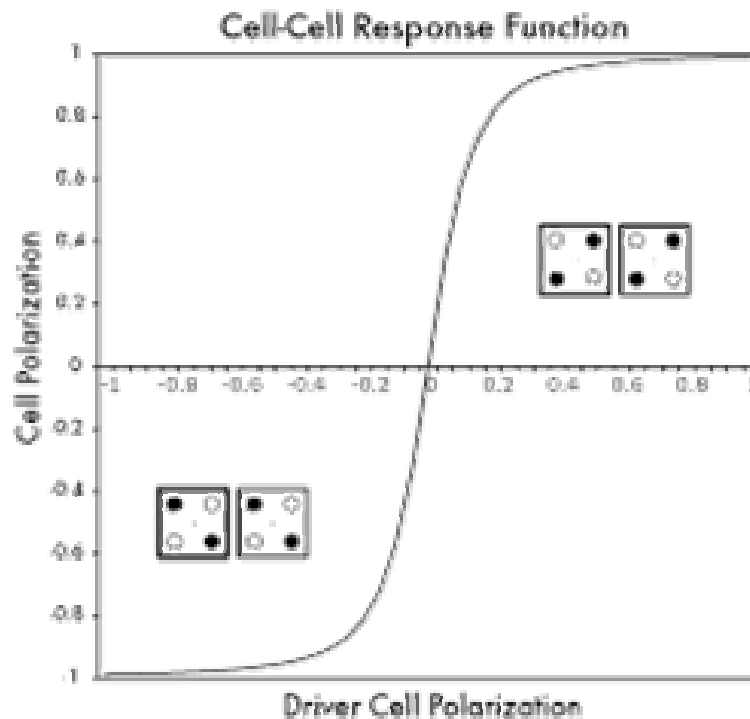


QCA cells showing the four quantum dots arranged in a square pattern.

(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- Electrons in cells placed adjacent to each other will interact.
- Polarization of one cell will be directly affected by the polarization of neighbouring cells.
- The cell-to-cell response function is as follows:

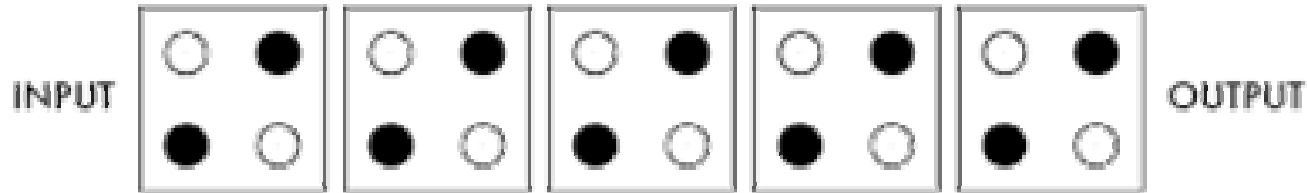


Non-linear response function of one cell onto its neighbour.

(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- Interaction forces neighbouring cells to synchronize their polarization.
- An array of QCA cells acts as a wire and is able to transmit information from one end to another.
- All the cells in the wire will switch their polarizations to follow that of the input or “driver” cell.

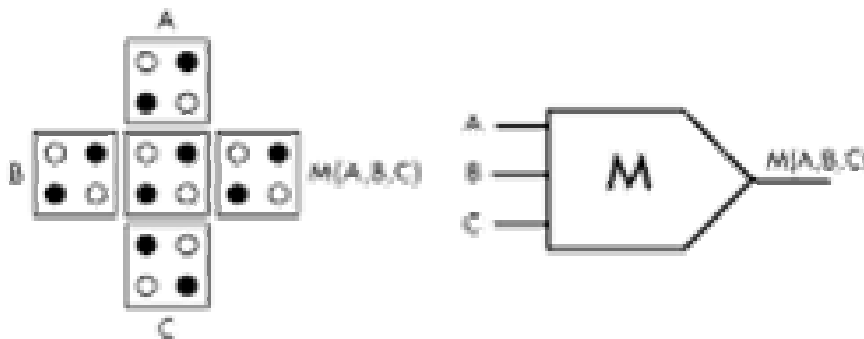


QCA cells lined up in this way create a QCA wire with short propagation delay

(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- How to create the basic Boolean logic gates (AND, OR, NOT)?
- Fundamental logic primitive that can be created with QCA is a *majority gate* or *majority voter*

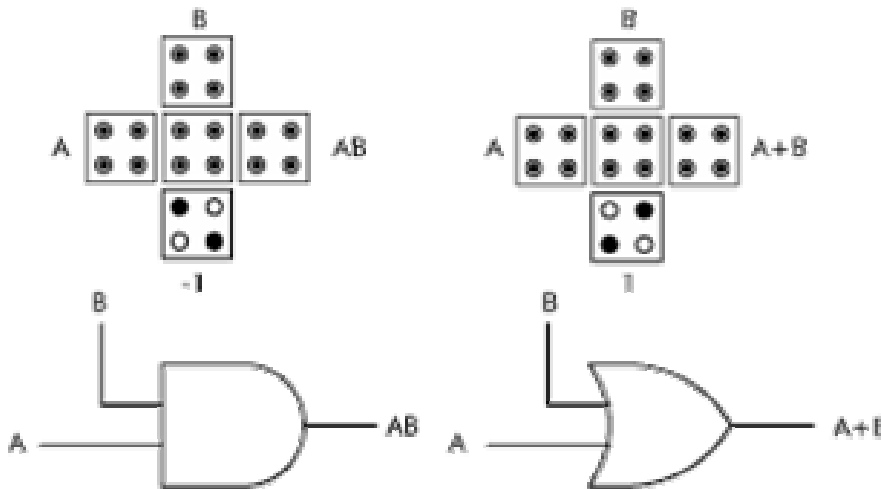


A	B	C	M
0	0	0	0
0	0	1	0
0	1	0	0
0	1	1	1
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	1

Majority gate with output reflecting majority of inputs
(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- In QCA, majority voter is the most fundamental gate
- Majority gate in CMOS would consist of several transistors
- With QCA, majority voter can be used in constructing AND and OR gates
- By fixing one of the inputs to the majority gate to 0 ($P = -1$) an AND gate can be created
- Fixing one of the inputs to 1 ($P = +1$), an OR gate is produced

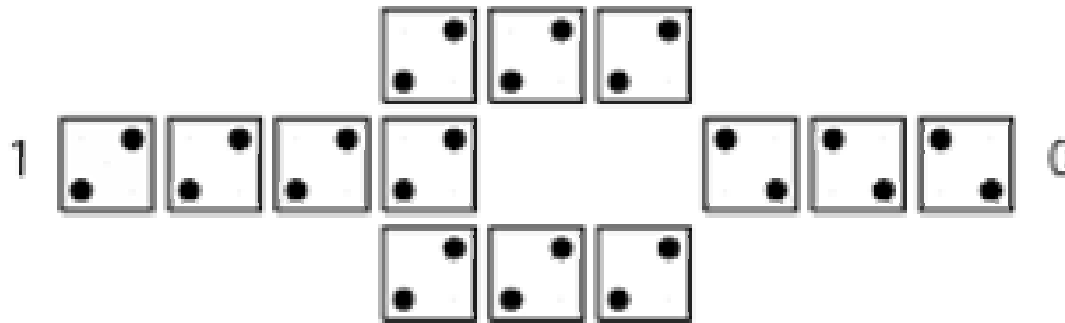


QCA AND and OR gates

(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- In QCA, the inverter is also simple to implement
- It has been empirically shown that two cells placed at 45 degrees with respect to each other interact *inversely*
- A possible inverter layout is as follows:

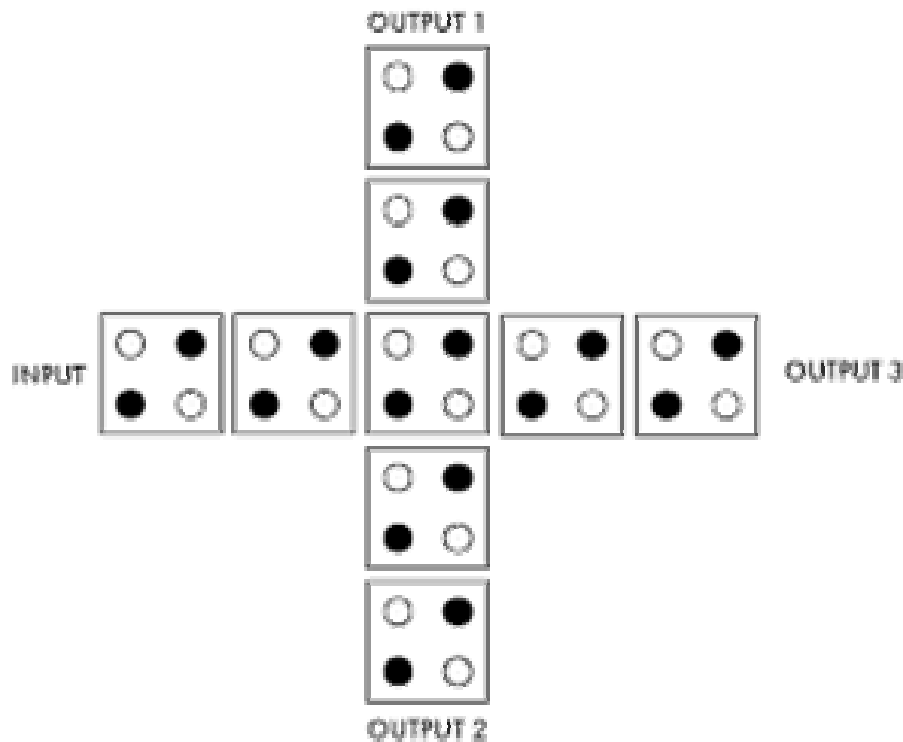


QCA inverter

(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- Fanout is another implementation to be looked at
- In standard electronic circuits a fanout is just a connection of several metal wires
- Implementing fanout in QCA is relatively simple
- Fanout is essentially a reversed majority voter

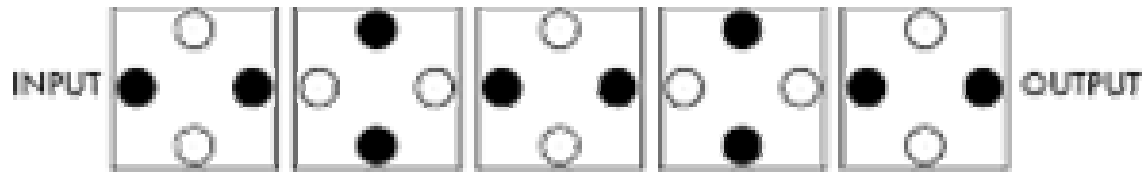


QCA fanout with input signal appearing at each of the outputs

(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- Another interesting possibility is an inverter chain
- Involves rotating dots by 45° (not placing at 45 degrees to each other like in the inverter)
- A wire created with these 45° cells forms an inverter chain where each cell takes on the opposite polarization of its neighbours

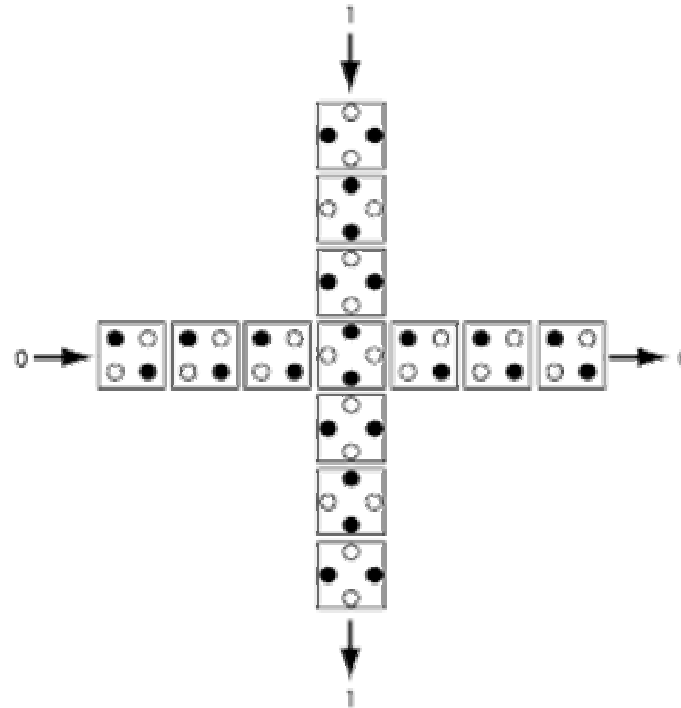


QCA inverter chain

(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- When a wire of regular cells crosses a wire of an inverter chain (45° cells) the two wires do not interact
- Thus signals can be crossed directly over each other as shown below:



QCA crossover

(Courtesy: Konrad Walus, University of Calgary)

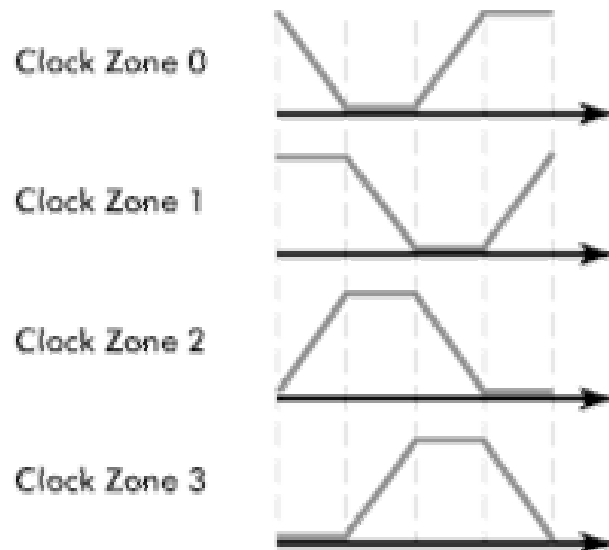


Quantum Cellular Automata

- Clocking is an important aspect of most computational technologies and a requirement for information flow in QCA.
- At this time all QCA circuit structures require a clock for synchronization and controlling of information flow as well as for power to run the circuit.
- QCA clocks have been proposed to control potential barriers between quantum dots.
- Control the rate at which electrons can quantum mechanically tunnel between dots and thus switch polarization.

Quantum Cellular Automata

- Clock signal high \rightarrow potential barriers between dots are LOW and electrons spread out in the cell with no net polarization ($P = 0$)
- Clock signal low \rightarrow potential barriers between dots are HIGH and electrons are localized such that a polarization is developed ($P = -1$ or $+1$) based on the interaction of their neighbors
- To pump information down a circuit in a controllable manner four clocking zones are usually available

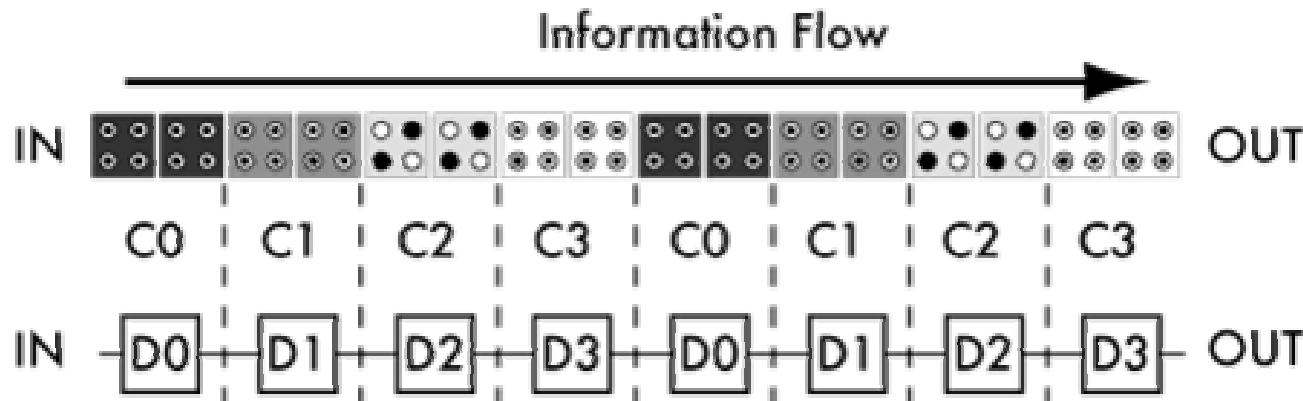


QCA clocking signals, with each clock lagging the previous signal by 90° in phase

(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- To pump information down a QCA wire, for example, different parts of the wire are connected to different clock signals.
- Since cells in one clock zone get latched and stay latched until the next group of cells get latched, they can be considered a D-latch.

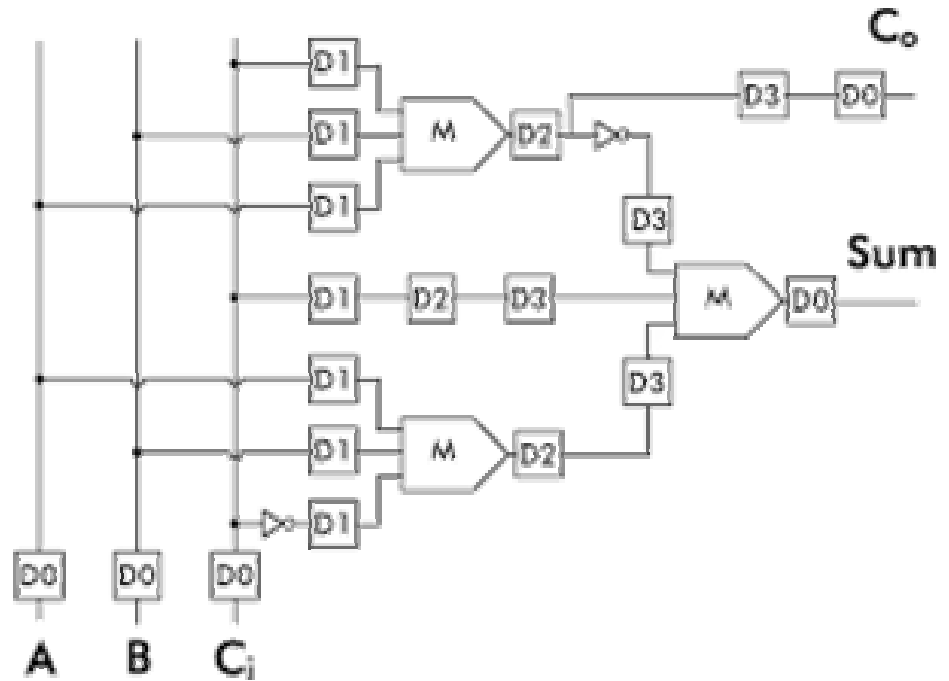
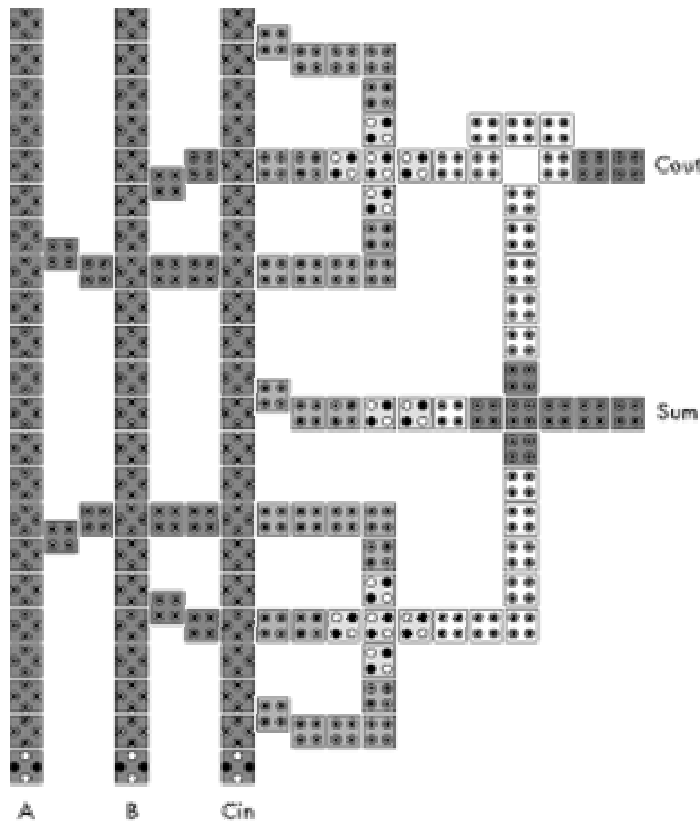


Clocked QCA Wire with information flowing from one clock zone to another

(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- The full adder is one of the most fundamental arithmetic building blocks.
- One of the first complex circuits design with QCA at Notre Dame
- Layout (left) and D-latch schematic (right) of a QCA full-adder:

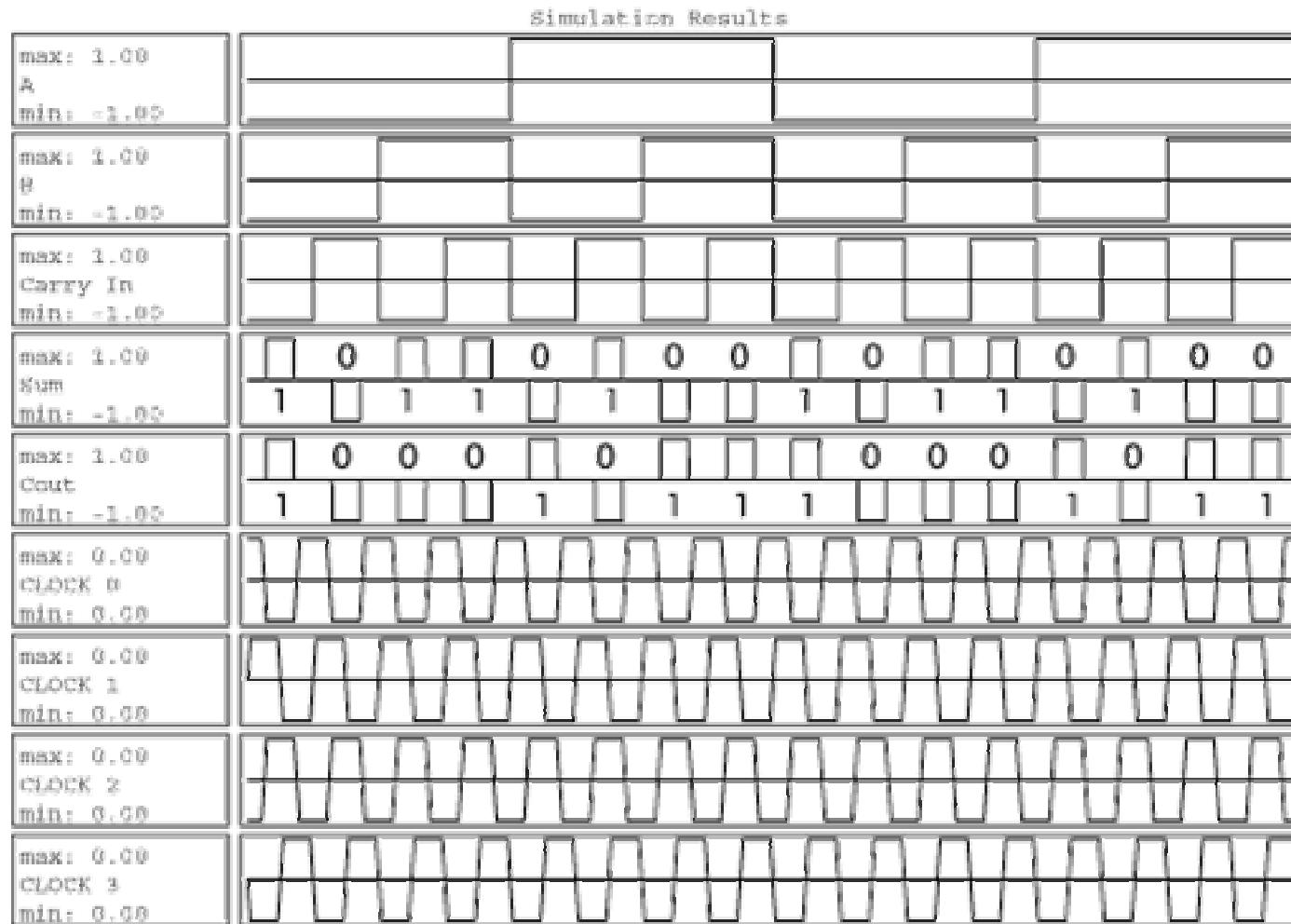


Quantum Cellular Automata

- Simulation results in QCADesigner bistable simulation engine developed at ATIPS Lab, University of Calgary
- First time outputs are latched, they fall to a random polarization not reflecting values of inputs, since they have not propagated through the circuit yet.
- One cycle delay between the time the inputs are set and when the outputs are latched
- Truth table of a full adder:

A	B	Cin	Sum	Cout
0	0	0	0	0
0	0	1	1	0
0	1	0	1	0
0	1	1	0	1
1	0	0	1	0
1	0	1	0	1
1	1	0	0	1
1	1	1	1	1

Quantum Cellular Automata



Simulation Results for a QCA Full Adder

(Courtesy: Konrad Walus, University of Calgary)

Quantum Cellular Automata

- Proposed implementations of QCA cells
 - Semiconductor
 - Advantageous because of the success of semiconductors in microelectronics → many tools and techniques have already been developed
 - Disadvantage is that dot size required to create room temperature devices is still outside the range of fabrication techniques
 - Molecular
 - Benefits from the high regularity of individual molecules and the small dot sizes available with molecules
 - Has potential to operate at room temperatures and at high operating speeds
 - Disadvantage is that placement of molecules required to create large circuits is probably still far off



Quantum Cellular Automata

- Magnetic
 - Uses nano-scale magnets to act as the cells and encodes the polarization in the magnetic vector of each of the nanomagnets
 - Within fabrication techniques and could operate at room temperature
 - However, does not appear to have necessary switching speed to compete with today's computers
 - May be useful in creating memory

Conclusions

- There is reasonable hope that quantum computers can one day be built.
- Currently only a 7 qubit computer has been built.
- There have been proposals to build quantum computers based on:
 - Nuclear magnetic resonance
 - Optical and solid-state technologies
 - Ion traps
- Quantum cellular automata is a novel idea which can take advantage of the quantum mechanical effects which occur at nanoscale dimensions.
- The quantum dots used in QCA are one of the most hopeful candidates for solid-state quantum computation with qubits.



References

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